Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Tunable Band Gap in Phosphorene Antidot Lattices ANDREW CUPO, Rensselaer Polytechnic Institute, PAUL MASIH DAS, GOPINATH DANDA, University of Pennsylvania, NEERAV KHARCHE, Rensselaer Polytechnic Institute, MARIJA DRNDIC, University of Pennsylvania, VINCENT MEUNIER, Rensselaer Polytechnic Institute — We used first-principles density functional theory (DFT) calculations to investigate the properties of phosphorene antidot lattices. It was found that the stability (quantified by the edge energy) decreases when the density of edges increases. This trend can be broken for H-passivated systems, where in some cases incrementing to a larger radius can increase stability. Most importantly, the band gap can be widely tuned through variation of the perforation spacing and radius. Moreover, deviations from the expected quantum confinement trends are not due to edge effects in general. Spatial distributions of the band gap are roughly bimodal with larger band gap atoms emanating from the zigzag edge, which can be explained by the presence of stronger quantum confinement effects in phosphorene nanoribbons with zigzag termination as compared to armchair termination. Transport will be favored along the armchair direction, which contains a continuous path of the lowest band gap atoms. A system with an electronic signature for metals has bands near the Fermi level that are localized to a new self-passivating 4x1 reconstruction of the zigzag edge and are flat (large effective mass), which suggest transport is not supported. The ability to tune phosphorene's band gap extends its applicability in optoelectronics.

Andrew Cupo
Rensselaer Polytechnic Institute

Date submitted: 10 Nov 2016

Electronic form version 1.4